



## LMCTEP: software for crystal-structure representation

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### ► To cite this version:

Alain Soyer. LMCTEP: software for crystal-structure representation. Journal of Applied Crystallography, 1993, 26 (3), pp.495. 10.1107/S0021889892010343 . hal-01214826

**HAL Id: hal-01214826**

**<https://hal.science/hal-01214826>**

Submitted on 5 Nov 2015

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*J. Appl. Cryst.* (1993). **26**, 495

**LMCTEP: software for crystal-structure representation.** By ALAIN SOYER, *Laboratoire de Minéralogie-Cristallographie, Unité associée au CNRS 09, Université Paris VI et Paris VII, Tour 16, Case 115, 4 place Jussieu, 75252 Paris CEDEX 05, France*

(Received 29 September 1992; accepted 2 October 1992)

**The crystallographic problem:** This software is intended for the space-filling representation of crystal structures. The first version (Soyer & Rimsky, 1992) did not have facilities for the extraction of data from a crystallographic information file (CIF) (Hall, Allen & Brown, 1991) or for the display of results on an X-Window terminal. The purpose of this Abstract is to announce a new version in which these facilities are available.

The software consists of two parts. The main part contains four mandatory programs and three utility programs. The second part consists of versions for X-Window terminals.

**Mandatory programs.** *GENER4* generates atomic positions in the cell starting from the asymmetric unit and the generator symmetry elements of the space group. *ORTHON* computes the contents of a 'piece' of crystal, with bonds if desired. *LMCTEP* computes a realistic shaded color image in true perspective, with spheres or ellipsoids representing atoms and cylinders representing bonds. *COLORT* is a small program that creates RGB color maps for the images.

**Utility programs.** *UTIPDB* extracts data from a Protein Data Bank file for visualization of the protein with *LMCTEP*. *UTILMC* reads a list of atoms and creates data files for visualization with *LMCTEP*. *UTICIF* extracts data from a CIF (see below).

The second part. *AFFICH* is a simple program that displays an image, calculated by *LMCTEP* using a color map created by *COLORT*, on an X-Window color display. *XMAFFICH* displays

several images, calculated by *LMCTEP* using color maps created by *COLORT*, on an X-Window color display. *XMLCTEP* is a full integrated version for X-Window terminals (see below).

**Method of solution:** The first version of the software has been described in detail (Soyer & Rimsky, 1992). Small modifications in the data-file format have now been made and some bugs have been removed. Two additional programs are available.

**UTICIF.** This is a utility program that extracts data from a crystallographic information file and creates the data files needed by our software; these files are filled with reasonable default values and may be modified later by means of a text editor.

**XMLCTEP.** This large program involves an OSF-Motif menu interface. Instead of creating data files with an editor and executing the programs sequentially, the user clicks on buttons and moves sliders with a mouse to choose options and values. All sequences that previously involved the mandatory programs are initiated from the menu. This program, written in C, is designed for Unix workstations and X-Window color displays.

**Software environment:** The main part of the software, written in Fortran77, is normally system independent and needs no extra software. The additional part, written in C, runs under Unix with the X-Window system and OSF-Motif widgets, so the Xlib, XtIntrinsic and Xm libraries are mandatory.

**Hardware environment:** The software runs on a Hewlett-Packard 9000/370 workstation (HP). The Fortran part is portable onto any computer that can address about 2 Mbytes of memory. A color screen with a depth of 8 bits (or more) is necessary to display the calculated image. The part of the program written in C needs more memory; 8 Mbytes are recommended.

**Program specifications:** Examples of run times have been given elsewhere (Soyer & Rimsky, 1992); note that modern RISC workstations are five to ten times as fast as our old HP. The volume of the source code can be estimated at 8000 lines (including commentaries), for both the Fortran and the C parts.

**Documentation:** The documentation of the first version was very brief and was incomplete. A new one, of about 700 lines, which describes the software organization, the installation procedure and the use of the main programs is now available in the form of an ASCII file. It contains sample data files and a listing of a typical execution.

**Availability:** This software is available on request from the author, whose email address is [soyer@lmcp.jussieu.fr](mailto:soyer@lmcp.jussieu.fr). The provision includes all source code, documentation and an example of some data files, and the preferred method of distribution is by email. If this is not possible, a 3.5 in MS-DOS diskette should be sent. Distribution is free of charge to the research and teaching communities.

**Keywords:** Crystal-structure representation, thermal ellipsoid, realistic synthetic image, CIF.

## References

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